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Infrared Spectroscopy with ab initio molecular dynamics simulations : gas phase floppy peptides of increasing size and complexity, in relation with IR-MPD experiments MARIE-PIERRE GAIGEOT, Universite d'Evry val d'Essonne - LAMBE UMR8587 , IR-MPD EXPS, GILLES GREGOIRE & J.P. SCHERMANN COLLABORATION, IR-MPD EXPS, L. SNOEK & T. VADEN COLLABORATION — We present finite temperature DFT-based Car-Parrinello molecular dynamics (MD) simulations for the calculation of infrared spectra of complex molecular systems, either in the gas phase or in the condensed phase. We will review the fundamentals of the method, as well as the applicability and originality of finite temperature MD simulations for the purpose of modeling infrared spectra. Illustrations are taken from the infrared spectroscopy of alanine peptides of increasing size and complexity (from dipeptides to an octo-peptide) in the gas phase, in relation with IR-MPD (Infrared Multi Photon Dissociation) experiments : 300-400 K gas-phase action spectroscopy as devised on the CLIO platform at the University of Orsay-France or on the platform developed in the group of L. Snoek at Oxford-UK. A special emphasis on vibrational anharmonicities and how they can be extracted from molecular dynamics simulations will be put forward. Furthermore, band assignments in terms of atomic movements from MD is challenging and we have introduced a general method for obtaining effective normal modes of molecular systems from MD simulations.

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